The Chemical Mechanism of MECCA used for the GABRIEL box model calculations in the accompanying paper

based on Sander et al. (2005)

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Table 1: Gas phase reactions

#	labels	reaction	rate constant	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.2E-11*EXP(70./temp)`	Sander et al. (2003)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	`6.E-34*((temp/300.)**(-2.4))*cair`	Sander et al. (2003)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	`k_3rd(temp,cair,5.7E-32,1.6,7.5E-11,0., 0.6)`	Sander et al. (2003)
G2104	StTrG	$OH + O_3 \rightarrow HO_2$	`1.7E-12*EXP(-940./temp)`	Sander et al. (2003)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	`5.5E-12*EXP(-2000./temp)`	Sander et al. (2003)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH$	`1.E-14*EXP(-490./temp)`	Sander et al. (2003)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O$	`4.8E-11*EXP(250./temp)`	Sander et al. (2003)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2$	`k_HO2_HO2`	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	`2.2E-10`	Sander et al. (2003)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	`2.9E-12*EXP(-160./temp)`	Sander et al. (2003)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`1.8E-11*EXP(110./temp)`	Sander et al. (2003)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	`3.E-12*EXP(-1500./temp)`	Sander et al. (2003)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	`1.2E-13*EXP(-2450./temp)`	Sander et al. (2003)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	`1.5E-11*EXP(170./temp)`	Sander et al. (2003)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	`k_NO3_NO2`	Sander et al. (2003)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	`k_NO3_NO2/(3.E-27*EXP(10990./temp))`	Sander et al. (2003)*
G3200	TrG	$NO + OH \rightarrow HONO$	`k_3rd(temp,cair,7.E-31,2.6,3.6E-11,0.1, 0.6)`	Sander et al. (2003)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	`3.5E-12*EXP(250./temp)`	Sander et al. (2003)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	`k_3rd(temp,cair,2.E-30,3.,2.5E-11,0., 0.6)`	Sander et al. (2003)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	`k_NO2_HO2`	Sander et al. (2003)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate constant	reference
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	`3.5E-12`	Sander et al. (2003)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	`1.8E-11*EXP(-390./temp)`	Sander et al. (2003)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	`k_HNO3_OH`	Sander et al. (2003)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	`k_NO2_HO2/(2.1E-27*EXP(10900./temp))`	Sander et al. (2003)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	`1.3E-12*EXP(380./temp)`	Sander et al. (2003)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	`1.85E-20*EXP(2.82*log(temp)-987./temp)`	Atkinson (2003)*
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	`7.3E-12*EXP(-620./temp)`	Sander et al. (2003)
G4103a	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH$	`4.1E-13*EXP(750./temp)/(1.+1./497.7*EXP(1160./temp))`	Sander et al. (2003)*
G4103b	StTrG	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	`4.1E-13*EXP(750./temp)/(1.+497.7*EXP(-1160./temp))`	Sander et al. (2003)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	`2.8E-12*EXP(300./temp)`	Sander et al. (2003)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	`1.3E-12`	Atkinson et al. (1999)
G4106a	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow 2\ HCHO + 2\ HO_2$	`9.5E-14*EXP(390./temp)/(1.+1./26.2*EXP(1130./temp))`	Sander et al. (2003)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH$	`9.5E-14*EXP(390./temp)/(1.+26.2*EXP(-1130./temp))`	Sander et al. (2003)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	`k_CH3OOH_OH`	Sander et al. (2003)*
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	`9.52E-18*EXP(2.03*log(temp)+636./temp)`	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	`3.4E-13*EXP(-1900./temp)`	Sander et al. (2003)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	`1.57E-13+cair*3.54E-33`	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow HO_2$	`4.E-13`	Sander et al. (2003)
G4200	TrGC	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	`1.49E-17*temp*temp*EXP(-499./temp)`	Atkinson (2003)
G4201	TrGC	$C_2H_4 + O_3 \rightarrow HCHO + .22\ HO_2 + .12\ OH + .23\ CO + .54\ HCOOH + .1\ H_2$	`1.2E-14*EXP(-2630./temp)`	Sander et al. (2003)*
G4202	TrGC	$C_2H_4 + OH \rightarrow .6666667\ CH_3CH(O_2)CH_2OH$	`k_3rd(temp,cair,1.E-28,0.8,8.8E-12,0.,0.6)`	Sander et al. (2003)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	`7.5E-13*EXP(700./temp)`	Sander et al. (2003)
G4204	TrGNC	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	`2.6E-12*EXP(365./temp)`	Sander et al. (2003)
G4205	TrGNC	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	`2.3E-12`	Atkinson et al. (1999)
G4206	TrGC	$C_2H_5O_2 + CH_3O_2 \rightarrow .75\ HCHO + HO_2 + .75\ CH_3CHO + .25\ CH_3OH$	`1.6E-13*EXP(195./temp)`	see note
G4207	TrGC	$C_2H_5OOH + OH \rightarrow .3\ C_2H_5O_2 + .7\ CH_3CHO + .7\ OH$	`k_CH3OOH_OH`	see note
G4208	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	`5.6E-12*EXP(270./temp)`	Sander et al. (2003)
G4209	TrGNC	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	`1.4E-12*EXP(-1900./temp)`	Sander et al. (2003)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate constant	reference
G4210	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2$	`4.E-13*EXP(200./temp)`	Sander et al. (2003)
G4211a	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	`4.3E-13*EXP(1040./temp)/(1.+1./37.*EXP(660./temp))`	Tyndall et al. (2001)
G4211b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	`4.3E-13*EXP(1040./temp)/(1.+37.*EXP(-660./temp))`	Tyndall et al. (2001)
G4212	TrGNC	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + NO_2$	`8.1E-12*EXP(270./temp)`	Tyndall et al. (2001)
G4213	TrGNC	$CH_3C(O)OO + NO_2 \rightarrow$ PAN	`k_PA_NO2`	Tyndall et al. (2001)
G4214	TrGNC	$CH_3C(O)OO + NO_3 \rightarrow CH_3O_2 + NO_2$	`4.E-12`	Canosa-Mas et al. (1996)
G4215a	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow HCHO + HO_2 + CH_3O_2 + CO_2$	`0.9*2.E-12*EXP(500./temp)`	Sander et al. (2003)
G4215b	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO + CO_2$	`0.1*2.E-12*EXP(500./temp)`	Sander et al. (2003)
G4216	TrGC	$CH_3C(O)OO + C_2H_5O_2 \rightarrow .82\ CH_3O_2 + CH_3CHO + .82\ HO_2 + .18\ CH_3COOH$	`4.9E-12*EXP(211./temp)`	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
G4217	TrGC	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	`2.5E-12*EXP(500./temp)`	Tyndall et al. (2001)
G4218	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO$	`k_CH3OOH_OH`	see note
G4219	TrGNC	NACA $+ OH \rightarrow NO_2 + HCHO + CO$	`5.6E-12*EXP(270./temp)`	see note
G4220	TrGNC	PAN $+ OH \rightarrow HCHO + NO_2$	`2.E-14`	see note
G4221	TrGNC	PAN $\rightarrow CH_3C(O)OO + NO_2$	`k_PAN_M`	Sander et al. (2003)*
G4300	TrGC	$C_3H_8 + OH \rightarrow .82\ C_3H_7O_2 + .18\ C_2H_5O_2 + H_2O$	`1.65E-17*temp*temp*EXP(-87./temp)`	Atkinson (2003)
G4301	TrGC	$C_3H_6 + O_3 \rightarrow .57\ HCHO + .47\ CH_3CHO + .33\ OH + .26\ HO_2 + .07\ CH_3O_2 + .06\ C_2H_5O_2 + .23\ CH_3C(O)OO + .04\ CH_3COCHO + .06\ CH_4 + .31\ CO + .22\ HCOOH + .03\ CH_3OH$	`6.5E-15*EXP(-1900./temp)`	Sander et al. (2003)*
G4302	TrGC	$C_3H_6 + OH \rightarrow CH_3CH(O_2)CH_2OH$	`k_3rd(temp,cair,8.E-27,3.5,3.E-11,0.,0.5)`	Atkinson et al. (1999)
G4303	TrGNC	$C_3H_6 + NO_3 \rightarrow$ ONIT	`4.6E-13*EXP(-1155./temp)`	Atkinson et al. (1999)
G4304	TrGC	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$	`k_PrO2_HO2`	Atkinson (1997)*
G4305	TrGNC	$C_3H_7O_2 + NO \rightarrow .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ C_3H_7ONO_2$	`k_PrO2_NO`	Atkinson et al. (1999)*
G4306	TrGC	$C_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3 + .8\ HCHO + .8\ HO_2 + .2\ CH_3OH$	`k_PrO2_CH3O2`	Kirchner and Stockwell (1996)
G4307	TrGC	$C_3H_7OOH + OH \rightarrow .3\ C_3H_7O_2 + .7\ CH_3COCH_3 + .7\ OH$	`k_CH3OOH_OH`	see note
G4308	TrGC	$CH_3CH(O_2)CH_2OH + HO_2 \rightarrow C_3H_6OOH$	`6.5E-13*EXP(650./temp)`	Müller and Brasseur (1995)
G4309	TrGNC	$CH_3CH(O_2)CH_2OH + NO \rightarrow .98\ CH_3CHO + .98\ HCHO + .98\ HO_2 + .98\ NO_2 + .02$ ONIT	`4.2E-12*EXP(180./temp)`	Müller and Brasseur (1995)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate constant	reference
G4310	TrGC	C_3H_6OOH + OH → .5 $CH_3CH(O_2)CH_2OH$ + .5 CH_3COCH_2OH + .5 OH + H_2O	`3.8E-12*EXP(200./temp)`	Müller and Brasseur (1995)
G4311	TrGC	CH_3COCH_3 + OH → $CH_3COCH_2O_2$ + H_2O	`1.33E-13+3.82E-11*EXP(-2000./temp)`	Sander et al. (2003)
G4312	TrGC	$CH_3COCH_2O_2$ + HO_2 → $CH_3COCH_2O_2H$	`8.6E-13*EXP(700./temp)`	Tyndall et al. (2001)
G4313	TrGNC	$CH_3COCH_2O_2$ + NO → NO_2 + $CH_3C(O)OO$ + HCHO	`2.9E-12*EXP(300./temp)`	Sander et al. (2003)
G4314	TrGC	$CH_3COCH_2O_2$ + CH_3O_2 → .5 CH_3COCHO + .5 CH_3OH + .3 $CH_3C(O)OO$ + .8 HCHO + .3 HO_2 + .2 CH_3COCH_2OH	`7.5E-13*EXP(500./temp)`	Tyndall et al. (2001)
G4315	TrGC	$CH_3COCH_2O_2H$ + OH → .3 $CH_3COCH_2O_2$ + .7 CH_3COCHO + .7 OH	`k_CH3OOH_OH`	see note
G4316	TrGC	CH_3COCH_2OH + OH → CH_3COCHO + HO_2	`3.E-12`	Atkinson et al. (1999)
G4317	TrGC	CH_3COCHO + OH → $CH_3C(O)OO$ + CO	`8.4E-13*EXP(830./temp)`	Tyndall et al. (1995)
G4318	TrGNC	MPAN + OH → CH_3COCH_2OH + NO_2	`3.2E-11`	Orlando et al. (2002)
G4319	TrGNC	MPAN → MVKO2 + NO_2	`k_PAN_M`	see note
G4320	TrGNC	$C_3H_7ONO_2$ + OH → CH_3COCH_3 + NO_2	`6.2E-13*EXP(-230./temp)`	Atkinson et al. (1999)
G4400	TrGC	C_4H_{10} + OH → $C_4H_9O_2$ + H_2O	`1.81E-17*temp*temp*EXP(114./temp)`	Atkinson (2003)
G4401	TrGC	$C_4H_9O_2$ + CH_3O_2 → .88 $CH_3COC_2H_5$ + .68 HCHO + 1.23 HO_2 + .12 CH_3CHO + .12 $C_2H_5O_2$ + .18 CH_3OH	`k_PrO2_CH3O2`	see note
G4402	TrGC	$C_4H_9O_2$ + HO_2 → C_4H_9OOH	`k_PrO2_HO2`	see note
G4403	TrGNC	$C_4H_9O_2$ + NO → .84 NO_2 + .56 $CH_3COC_2H_5$ + .56 HO_2 + .28 $C_2H_5O_2$ + .84 CH_3CHO + .16 ONIT	`k_PrO2_NO`	see note
G4404	TrGC	C_4H_9OOH + OH → .15 $C_4H_9O_2$ + .85 $CH_3COC_2H_5$ + .85 OH + .85 H_2O	`k_CH3OOH_OH`	see note
G4405	TrGC	MVK + O_3 → .45 HCOOH + .9 CH_3COCHO + .1 $CH_3C(O)OO$ + .19 OH + .22 CO + .32 HO_2	`.5*(1.36E-15*EXP(-2112./temp) +7.51E-16*EXP(-1521./temp))`	Pöschl et al. (2000)
G4406	TrGC	MVK + OH → MVKO2	`.5*(4.1E-12*EXP(452./temp) +1.9E-11*EXP(175./temp))`	Pöschl et al. (2000)
G4407	TrGC	MVKO2 + HO_2 → MVKOOH	`1.82E-13*EXP(1300./temp)`	Pöschl et al. (2000)
G4408	TrGNC	MVKO2 + NO → NO_2 + .25 $CH_3C(O)OO$ + .25 CH_3COCH_2OH + .75 HCHO + .25 CO + .75 HO_2 + .5 CH_3COCHO	`2.54E-12*EXP(360./temp)`	Pöschl et al. (2000)
G4409	TrGNC	MVKO2 + NO_2 → MPAN	`.25*k_3rd(temp,cair,9.7E-29,5.6, 9.3E-12,1.5,0.6)`	Pöschl et al. (2000)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate constant	reference
G4410	TrGC	MVKO2 + CH_3O_2 → .5 CH_3COCHO + .375 CH_3COCH_2OH + .125 $CH_3C(O)OO$ + 1.125 HCHO + .875 HO_2 + .125 CO + .25 CH_3OH	`2.E-12`	von Kuhlmann (2001)
G4411	TrGC	MVKO2 + MVKO2 → CH_3COCH_2OH + CH_3COCHO + .5 CO + .5 HCHO + HO_2	`2.E-12`	Pöschl et al. (2000)
G4412	TrGC	MVKOOH + OH → MVKO2	`3.E-11`	Pöschl et al. (2000)
G4413	TrGC	$CH_3COC_2H_5$ + OH → MEKO2	`1.3E-12*EXP(-25./temp)`	Atkinson et al. (1999)
G4414	TrGC	MEKO2 + HO_2 → MEKOOH	`k_PrO2_HO2`	see note
G4415	TrGNC	MEKO2 + NO → .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 ONIT	`k_PrO2_NO`	see note
G4416	TrGC	MEKOOH + OH → .8 MeCOCO + .8 OH + .2 MEKO2	`k_CH3OOH_OH`	see note
G4417	TrGNC	ONIT + OH → $CH_3COC_2H_5$ + NO_2 + H_2O	`1.7E-12`	Atkinson et al. (1999)*
G4500	TrGC	ISOP + O_3 → .28 HCOOH + .65 MVK + .1 MVKO2 + .1 $CH_3C(O)OO$ + .14 CO + .58 HCHO + .09 H_2O_2 + .08 CH_3O_2 + .25 OH + .25 HO_2	`7.86E-15*EXP(-1913./temp)`	Pöschl et al. (2000)
G4501	TrGC	ISOP + OH → ISO2	`2.54E-11*EXP(410./temp)`	Pöschl et al. (2000)
G4502	TrGNC	ISOP + NO_3 → ISON	`3.03E-12*EXP(-446./temp)`	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO_2 → ISOOH	`2.22E-13*EXP(1300./temp)`	Boyd et al. (2003)*
G4504	TrGNC	ISO2 + NO → .956 NO_2 + .956 MVK + .956 HCHO + .956 HO_2 + .044 ISON	`2.54E-12*EXP(360./temp)`	Pöschl et al. (2000)*
G4505	TrGC	ISO2 + CH_3O_2 → .5 MVK + 1.25 HCHO + HO_2 + .25 CH_3COCHO + .25 CH_3COCH_2OH + .25 CH_3OH	`2.E-12`	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 → 2 MVK + HCHO + HO_2	`2.E-12`	Pöschl et al. (2000)
G4507	TrGC	ISOOH + OH → MVK + OH	`1.E-10`	Pöschl et al. (2000)
G4508	TrGNC	ISON + OH → CH_3COCH_2OH + NACA	`1.3E-11`	Pöschl et al. (2000)

*Notes:

G1002: path leading to 2 $O(^3P)$ + O_2 neglected

G2108: branching ratio from Hack et al., see note B5 of Sander et al. (2003)

G2110: The rate constant is: `k_HO2_HO2 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*zcon)*(1.0_dp+1.4E-21*EXP(2200./temp)*C(KPP_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984)

G3109: The rate constant is: `k_NO3_NO2 = k_3rd(temp,zcon,2.0E-30,4.4,1.4E-12,0.7,0.6)`.

G3110: The rate constant is defined as backward reaction divided by equilibrium constant.

G3206: The rate constant is: `k_HNO3_OH = 2.4E-14*EXP(460./temp)+1./((1./6.5E-34*EXP(1335./temp)*zcon)+(1./2.7E-17*EXP(2199./temp)))`

G3207: The rate constant is defined as backward reaction divided by equilibrium constant.

G4103: product distribution is from Elrod et al. (2001)

G4107: The rate constant is: `k_CH3OOH_OH = 3.8E-12*EXP(200./temp)`

G4109: same temperature dependence assumed as for $CH_3CHO+NO_3$

G4201: product distribution is from von Kuhlmann (2001) (see also Neeb et al. (1998))

G4206: Rate coefficient calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH_3OO and C_2H_5OO from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution (branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

G4207: same value as for G4107: $CH_3OOH+OH$ assumed

G4213: The rate constant is: `k_PA_NO2` = `k_3rd(temp, zcon,8.5E-29,6.5,1.1E-11,1.0,0.6)`.

G4216: `1.0E-11` from Atkinson et al. (1999), temperature dependence from Kirchner and Stockwell (1996)

G4218: same value as for G4107: $CH_3OOH+OH$ assumed

G4219: according to Pöschl et al. (2000), the same value as for $CH_3CHO+OH$ can be assumed

G4220: 50% of the upper limit given by Sander et al. (2003), as suggested by von Kuhlmann (2001)

G4221: The rate constant is: `k_PAN_M` = `k_PA_NO2/ 9.E-29*EXP(-14000./temp)`, i.e. the rate constant is defined as backward reaction divided by equilibrium constant.

G4301: product distribution is for terminal olefin carbons from Zaveri and Peters (1999)

G4304: The rate constant is: `k_PrO2_HO2` = `1.9E-13*EXP(1300./temp)`. Value for generic RO_2 + HO_2 reaction from Atkinson (1997) is used.

G4305: The rate constant is: `k_PrO2_NO` = `2.7E-12*EXP(360./temp)`

G4306: The rate constant is: `k_PrO2_CH3O2` = `9.46E-14*EXP(431./temp)`. The product distribution is from von Kuhlmann (2001).

G4307: same value as for G4107: $CH_3OOH+OH$ assumed

G4309: products are from von Kuhlmann (2001)

G4315: same value as for G4107: $CH_3OOH+OH$ assumed

G4319: same value as for PAN assumed

G4401: same value as for propyl group assumed (`k_PrO2_CH3O2`)

G4402: same value as for propyl group assumed (`k_PrO2_HO2`)

G4403: same value as for propyl group assumed (`k_PrO2_NO`)

G4404: same value as for G4107: $CH_3OOH+OH$ assumed

G4409: The factor 0.25 was recommended by Uli Poeschl (pers. comm. 2004).

G4414: same value as for propyl group assumed (`k_PrO2_HO2`)

G4415: same value as for propyl group assumed (`k_PrO2_NO`)

G4416: same value as for G4107: $CH_3OOH+OH$ assumed

G4417: value for $C_4H_9ONO_2$ used here

G4503: same temperature dependence assumed as for other RO_2+HO_2 reactions

G4504: Yield of 12 % $RONO_2$ assumed as suggested in Table 2 of Sprengnether et al. (2002).

Table 2: Photolysis reactions

#	labels	reaction	rate constant	reference
J1001a	StTrGJ	O_3 + hν → O(^{1}D)	J_O1D	see note
J1001b	StTrGJ	O_3 + hν → O(^{3}P)	J_O3P	see note
J2101	StTrGJ	H_2O_2 + hν → 2 OH	J_H2O2	see note
J3101	StTrGNJ	NO_2 + hν → NO + O(^{3}P)	J_NO2	see note
J3103a	StTrGNJ	NO_3 + hν → NO_2 + O(^{3}P)	J_NO2O	see note
J3103b	StTrGNJ	NO_3 + hν → NO	J_NOO2	see note
J3104	StTrGNJ	N_2O_5 + hν → NO_2 + NO_3	J_N2O5	see note
J3200	TrGJ	HONO + hν → NO + OH	J_HONO	see note
J3201	StTrGNJ	HNO_3 + hν → NO_2 + OH	J_HNO3	see note
J3202	StTrGNJ	HNO_4 + hν → .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH	J_HNO4	see note
J4100	StTrGJ	CH_3OOH + hν → HCHO + OH + HO_2	J_CH3OOH	see note
J4101a	StTrGJ	HCHO + hν → H_2 + CO	J_COH2	see note
J4101b	StTrGJ	HCHO + hν → H + CO + HO_2	J_CHOH	see note
J4200	TrGCJ	C_2H_5OOH + hν → CH_3CHO + HO_2 + OH	J_CH3OOH	see note
J4201	TrGCJ	CH_3CHO + hν → CH_3O_2 + HO_2 + CO	J_CH3CHO	see note
J4202	TrGCJ	$CH_3C(O)OOH$ + hν → CH_3O_2 + OH	J_PAH	see note
J4203	TrGNCJ	NACA + hν → NO_2 + HCHO + CO	0.19*J_CHOH	see note
J4204	TrGNCJ	PAN + hν → $CH_3C(O)OO$ + NO_2	J_PAN	see note
J4300	TrGCJ	C_3H_7OOH + hν → CH_3COCH_3 + HO_2 + OH	J_CH3OOH	see note
J4301	TrGCJ	CH_3COCH_3 + hν → $CH_3C(O)OO$ + CH_3O_2	J_CH3COCH3	see note
J4302	TrGCJ	CH_3COCH_2OH + hν → $CH_3C(O)OO$ + HCHO + HO_2	0.074*J_CHOH	see note
J4303	TrGCJ	CH_3COCHO + hν → $CH_3C(O)OO$ + CO + HO_2	J_CH3COCHO	see note
J4304	TrGCJ	$CH_3COCH_2O_2H$ + hν → $CH_3C(O)OO$ + HO_2 + OH	J_CH3OOH	see note
J4305	TrGNCJ	MPAN + hν → CH_3COCH_2OH + NO_2	J_PAN	see note
J4306	TrGNCJ	$C_3H_7ONO_2$ + hν → CH_3COCH_3 + NO_2 + HO_2	3.7*J_PAN	see note
J4400	TrGCJ	C_4H_9OOH + hν → OH + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	J_CH3OOH	see note
J4401	TrGCJ	MVK + hν → $CH_3C(O)OO$ + HCHO + CO + HO_2	0.019*J_COH2+.015*J_CH3COCHO	see note
J4402	TrGCJ	MVKOOH + hν → OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 $CH_3C(O)OO$ + .25 CO	J_CH3OOH	see note
J4403	TrGCJ	$CH_3COC_2H_5$ + hν → $CH_3C(O)OO$ + $C_2H_5O_2$	0.42*J_CHOH	see note
J4404	TrGCJ	MEKOOH + hν → $CH_3C(O)OO$ + CH_3CHO + OH	J_CH3OOH	see note
J4405	TrGCJ	MeCOCO + hν → 2 $CH_3C(O)OO$	2.15*J_CH3COCHO	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate constant	reference
J4406	TrGNCJ	ONIT + hν $\rightarrow$ NO_2 + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	3.7*J_PAN	see note
J4500	TrGCJ	ISOOH + hν $\rightarrow$ MVK + HCHO + HO_2 + OH	J_CH3OOH	see note
J4501	TrGNCJ	ISON + hν $\rightarrow$ MVK + HCHO + NO_2 + HO_2	3.7*J_PAN	see note

*Notes: J-values are calculated with the radiative transfer model TUV v4.1 (Madronich and Flocke, 1998) and then supplied to the MECCA chemistry.

Table 3: Notation used in MIM and MECCA v0.1p:

notation MECCA in Sander et al. (2005)	notation MIM in Pöschl et al. (2000)	species
ISOP	C_5H_8	isoprene
ISO2	ISO_2	peroxy radicals from $C_5H_8 + OH$
ISOOH	ISO_2H	β-hydroxyhydroperoxides from $ISO_2 + HO_2$
ISON	ISON	β-hydroxyalkylnitrates from $ISO_2 + NO$ and alkylnitrates from $C_5H_8 + NO_3$
MVK	MACR	methacrolein, methylvinylketone and other C_4 carbonyls
MVKO2	$MACRO_2$	peroxy radicals from MACR + OH
MVKOOH	$MACRO_2H$	hydroperoxides from $MACRO_2 + HO_2$
MPAN	MPAN	peroxymethacryloylnitrate and other higher peroxyacylnitrates
ACETOL	HACET	hydroxyacetone and other C_3 ketones
MGLO	MGLY	methylglyoxal and other C_3 aldehydes
PA	CH_3CO_3	peroxy acetyl radical
PAN	PAN	peroxy acetyl nitrate
PAA	CH_3CO_3H	peroxy acetic acid
CH3COOH	CH_3COOH	acetic acid
NACA	NALD	nitro-oxy acetaldehyde
HCOOH	HCOOH	formic acid

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